High end computing for nuclear fission science and engineering

Paul Meakin

Salt Lake City, Thursday February 23, 2005

Idaho National Laboratory

Group organizers

Group I: Computational fluid dynamics and transport:
Yassin Hassan, Department of Nuclear Engineering Texas A&M

Group II Computational materials science:

Sid Yip, Department of Nuclear Science and Engineering, MIT

Group III: Computational chemistry
David Dixon, Department of Chemistry, University of Alabama

Group E: Nuclear engineering and reactor physics:
Dmitriy Anistratov, Nuclear Engineering Department, North Carolina State University
Abderrafi Ougoaug, Nuclear Programs, Idaho National Laboratory
Paul Turinsky, Nuclear Engineering Department, North Carolina State University

DOE Computing Resources

Doug Kothe (ORNL): National Leadership Computing Facility (NLCF)

Francesca Verdier (LBL): National Energy Research Computing Center (NERSC)

Nuclear cross-sections

Ludovic Bonneau: Nuclear Physics Group, Los Alamos National Laboratory

Thomas Papenbrock: Physics Division, Oak Ridge National Laboratory

Argonne – IBM BlueGene System

- Joint OS/NE project
- ≈ 50% User facility for Global Nuclear Energy Partnership (GNEP)
- FY 2007 – 100Tf BlueGene/P
- FY 2008 – 500Tf BlueGene/P
- FY 2010 – 10Pf BlueGene/Q??
- Access Model??

Workshop Objectives

- Help ensure that the basic computational research needed to support the rebirth and future of nuclear fission energy in the United States is done in a timely manner.

- Help ensure that computational engineering science is used as effectively as possible to reduce the cost of developing advanced nuclear energy systems, compress the development timetable and optimize the overall performance (proliferation resistance, reliability, safety, sustainability, economics, waste reduction)

- This will not happen without access to high end computers and the development of the software needed to use them effectively.

Workshop Objectives

- Identify the computational domains that are the most critical to the nuclear fission energy enterprise and require high end computing to succeed.

- Lay the groundwork for future workshops that will focus on gaining access to high-end (Leadership Class) computing systems for the most promising applications identified in this workshop (opportunity for seminal scientific discovery, meets critical need(s) for nuclear fission energy programs, availability of code that makes effective use of current and planned machines).

- Make sure that computational engineering does not get left behind (high end computing is being used for applications such as accelerators, 'light' sources and fission energy system design).

Follow-on Workshop Criteria

• Enthusiasm – willingness to create a proposal team and supporting community to justify NLCF End Station.

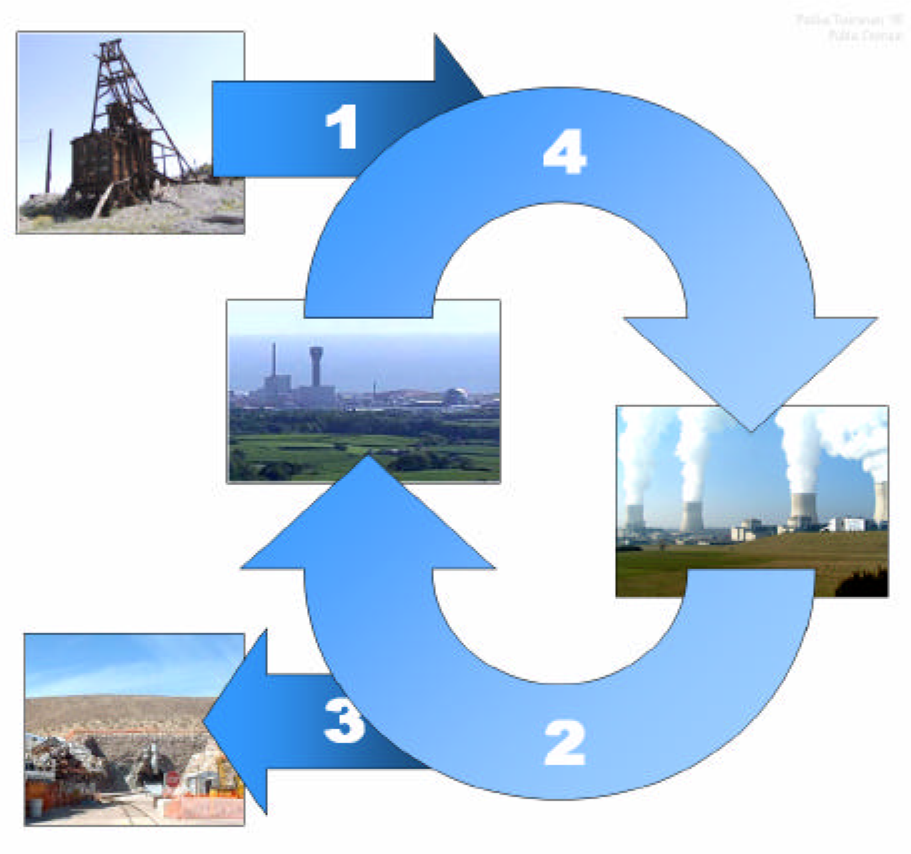
• Demonstrated need for high-end computing to achieve basic science breakthrough(s) essential to the future of nuclear energy.

• Availability of code ready to run (effectively) on NLCF (Cray) and/or other systems (Developmental End Station to generate code).

• Ability to satisfy NLCF criteria and develop competitive proposal.

Consider entire fuel cycle (every component must be optimized – it's not just reactors)

- Mining and fuel processing
- Burnup in reactor and energy generation
- Hydrogen production via thermochemical cycle or high temperature electrolysis
- Spent fuel separation and reprocessing
- Short term and long term (repository) storage.

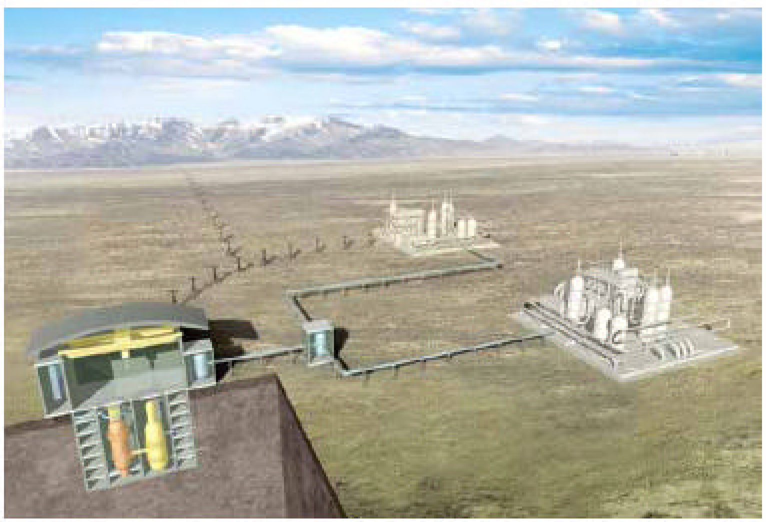


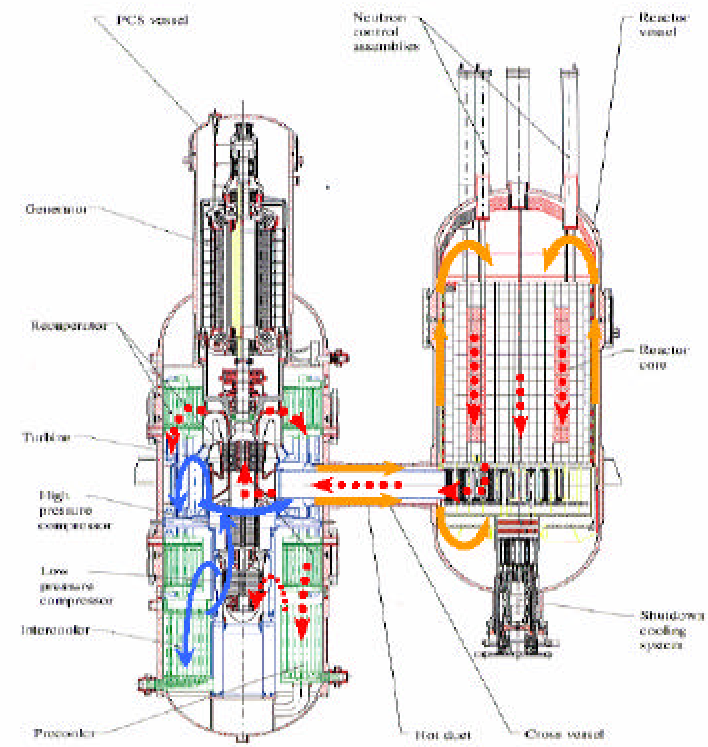
Very high temperature gas cooled reactor for hydrogen production - Next Generation Nuclear Plant (NGNP)

Chemistry: Catalyst stability

Materials: High temperatures, radiation effects, corrosion

Flow and transport: temperature distribution





General Atomics design of a block VHTR showing the power unit on the left and the reactor vessel on the right. The lower plenum is just below the core where the flow turns 90°.

Idaho National Laboratory